Adiabatic Conditions and the Uncertainty Relation

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(Dated: January 9, 2013)

The condition for adiabatic approximation are of basic importance for the applications of the adiabatic theorem. The traditional quantitative condition was found to be necessary but not sufficient, but we do not know its physical meaning and the reason why it is necessary from the physical point of view. In this work, we relate the adiabatic theorem to the uncertainty relation, and present a clear physical picture of the traditional quantitative condition. It is shown that the quantitative condition is just the amplitude of the probability of transition between two levels in the time interval which is of the order of the time uncertainty of the system. We also present a new sufficient condition with clear physical picture.

The adiabatic theorem [1, 2] is one of the basic results in quantum theory and has applications in many fields, for example, in quantum field theory [3], geometric phase [4] as well as in quantum control and adiabatic quantum computation [5]. As described in many publications, the traditional adiabatic theorem [6, 7] states that if a quantum system with a time-dependent Hamiltonian $\hat{H}(\mathbf{t})$ is initially in the n_th instantaneous eigenstate of $\hat{H}(0)$, $\hat{H}(\mathbf{t})$ evolves slowly enough and the energy levels don't cross in the evolution process, then the state of the system will stay at the n_th instantaneous eigenstate of $\hat{H}(\mathbf{t})$ up to a phase factor at a later time. But the application of the theorem depends on the criterion of the "slowness". Usually, the "slowness" is described as follows [8]

$$\left|\frac{\left\langle E_n\left(t\right)\right|\left.\dot{E}_m\left(t\right)\right\rangle}{E_m\left(t\right)-E_n\left(t\right)}\right|\ll 1, m\neq n, t\in[0,T] \tag{1}$$

where $E_n\left(t\right)$ and $\left|E_n\left(t\right)\right\rangle$ are the instantaneous eigenvalues and eigenstates of $\hat{H}\left(t\right)$, and T is the total evolution time.

In recent years, many doubts have been raised in the traditional criterion [8–12]. It was first shown by Marzlin and Sanders [8] and then by Tong et al [9] that if two systems which we call system S^A and S^B are related though

$$\hat{H}^B\left(t\right)=-\hat{U}^{A+}\left(t\right)\hat{H}^A\left(t\right)\hat{U}^A\left(t\right) \tag{2}$$

The two systems can't have an adiabatic evolution at the same time unless $\left|\left\langle E_n^A\left(t\right)\right|\left.E_n^A\left(0\right)\right\rangle\right|\approx 1$, even if both of the system satisfy condition (1). Many authors investigated the reasons of the insufficiency [13–16]. Recently, Amin pointed out that the violations of the traditional criterion all arise from resonant transitions between energy levels [11]. At the same time, some authors proposed some new alternative criterions [17–24]. In 2008, Du et al experimentally examined the traditional criterion [10].

However, the physical pictures of the criterions proposed before are not clear. Even though Tong proved that the traditional condition (1) is necessary in guaranteeing the validity of the adiabatic approximation [12], we still do not know the reason why it is necessary from the physical point of view. It is foundmentally important to find a new condition with clear physics picture or probe the physical meaning of the existed conditions. In this letter, we relate the adiabatic condition to the uncertainty relation. We first propose a new sufficient condition for adiabatic process, and then give clear physical pictures of the new condition and the necessary condition (1) in terms of the uncertainty relation. It is shown that the state of a system cannot be appreciably modified by an evolution until a least evolution time has elapsed, and $\left|\frac{\left\langle E_n(t)\right|\left.\dot{E}_m(t)\right\rangle}{E_n(t)-E_m(t)}\right|$ in Eq. (1) is just the amplitude of the probability of the transition between $\left|E_n\left(t\right)\right\rangle$ and $\left|E_m\left(t\right)\right\rangle$ in the least evolution time. The least evolution time is of the order of the time-uncertainty of the system.

In an adiabatic process, if the system is initially in the n_th instantaneous eigenstate $\left|E_n\left(0\right)\right\rangle$, then at the end of the adiabatic evolution process the state $\left|\psi\left(t\right)\right\rangle$ fulfills

$$\left|\left\langle E_n\left(T\right)\mid\psi\left(T\right)\right\rangle\right|^2\approx 1. \tag{3}$$

Let

$$\left|\psi\left(t\right)\right\rangle=\sum_m a_m\left(t\right)\left|E_m\left(t\right)\right\rangle, \tag{4}$$

where $a_m\left(t\right)$ is a complex number. Substituting the above equation into the Schrödinger equation, we obtain

$$\frac{d}{dt}a_n\left(t\right)=-\sum_m a_m\left(t\right)\left\langle E_n\left(t\right)\right|\left.\dot{E}_m\left(t\right)\right\rangle-\frac{i}{\hbar}a_n\left(t\right)E_n\left(t\right) \tag{5}$$

and

$$\frac{d}{dt}a_n^*\left(t\right)=-\sum_m a_m^*\left(t\right)\left\langle\dot{E}_m\left(t\right)\right|\left.E_n\left(t\right)\right\rangle+\frac{i}{\hbar}a_n^*\left(t\right)E_n\left(t\right) \tag{6}$$

Using equations (5) and (6), and denoting $P_n(t)=$

$a_n(t)\,a_n^*(t)$, we have

$$\begin{aligned}\frac{d}{dt}P_n(t) &= a_n(t)\frac{d}{dt}a_n^*(t)+a_n^*(t)\frac{d}{dt}a_n(t)\\ &= -\sum_m a_n(t)\,a_m^*(t)\left\langle \dot{E}_m(t)\,\middle|\,E_n(t)\right\rangle\\ &\quad -\sum_m a_n^*(t)\,a_m(t)\left\langle E_n(t)\,\middle|\,\dot{E}_m(t)\right\rangle\\ &= -2\sum_m Re\left\{a_n^*(t)\,a_m(t)\,\chi_{nm}\right\} \qquad (7)\end{aligned}$$

where $\chi_{nm}=\left\langle E_n(t)\,\middle|\,\dot{E}_m(t)\right\rangle$, and we use a gauge in which $\chi_{nn}=0$. Integrating equation (7), we get

$$\begin{aligned}P_n(T) &= 1-2\sum_m\int_0^T Re(a_n(t)\,a_m^*(t)\,\chi_{nm})\,dt\\ &\geq 1-2\sum_{m\neq n}\int_0^T|\chi_{nm}|\,dt\\ &\geq 1-2\sum_{m\neq n}T\max\{|\chi_{nm}|\} \qquad (8)\end{aligned}$$

When the dimension of the system is finite, if we have

$$2T\max\left\{\left|\left\langle E_m(t)\,\middle|\,\dot{E}_n(t)\right\rangle\right|\right\}\ll 1, \qquad (9)$$

the sum in the equation (8) can always be a small number so that $P_n(T)\approx 1$, which means that condition (9) is a sufficient condition for adiabatic theorem.

Condition (9) can sufficiently guarantee the validity of the adiabatic approximation, but we do not understand its physical meaning clearly, just as we do with the necessary condition (1). Especially, condition (9) means seemingly that only if T is small enough and $\max\left\{\left|\left\langle E_m(t)\,\middle|\,\dot{E}_n(t)\right\rangle\right|\right\}$ is finite, it can always be fulfilled and the adiabatic approximation can be guaranteed. This conflicts seemingly with condition (1) in which the time T seems be not involved. How to attemper this conflict? Let's go to the central purpose of this letter, we will present the clear physical pictures of conditions (1) and (9). From these pictures conditions (1) and (9) are consistent. Interestingly, the uncertainty relation plays a key role here.

We first show that the evolution time must be more than the least evolution time to get an obvious state change, and the least evolution time is in the order of the time uncertainty of the system.

For simplicity, we consider a two level system. The Hamiltonian $\hat{H}(t)$ has two eigenstates $|E_k(t)\rangle$ and $|E_n(t)\rangle$ which satisfy the following equation

$$\hat{H}(t)\,|E_{n,k}(t)\rangle = E_{n,k}(t)\,|E_{n,k}(t)\rangle. \qquad (10)$$

The state of the system at time t, $|\psi(t)\rangle$, can be expanded as

$$|\psi(t)\rangle=\sum_n a_n(t)\,e^{i\beta_n(t)}\,|E_n(t)\rangle \qquad (11)$$

where $a_n(t)$ and $\beta_n(t)$ are real, and the phase $\beta_n(t)$ can be expressed as [25]

$$\beta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')dt'+i\int_0^t\left\langle E_n(t')\,\middle|\,\dot{E}_n(t')\right\rangle dt'. \qquad (12)$$

Substituting equations (11) and (12) into the Schrödinger equation, we obtain

$$\frac{da_k(t)}{dt}=-a_n(t)\,e^{i\beta_{nk}(t)}\left\langle E_k(t)\,\middle|\,\dot{E}_n(t)\right\rangle \qquad (13)$$

where $\beta_{nk}(t)=\beta_n(t)-\beta_k(t)$. Let us consider two systems S^A and S^B, the Hamiltonian of which are related though Eq. (2) as shown in [8, 9]. The instantaneous eigenvalues and eigenstates of the two system satisfy [9]

$$\begin{aligned}&E_n^B(t)=-E_n^A(t)\\ &\left|E_n^B(t)\right\rangle=\hat{U}^{A+}(t)\left|E_n^A(t)\right\rangle\end{aligned} \qquad (14)$$

and their evolution operator

$$\hat{U}^B(t)=\hat{U}^{A+}(t). \qquad (15)$$

From Eqs. (14) and (15) we have

$$\left\langle E_k^B(t)\,\middle|\,\dot{E}_n^B(t)\right\rangle=\frac{i}{\hbar}E_n^A(t)\,\delta_{nk}+\left\langle E_k^A(t)\,\middle|\,\dot{E}_n^A(t)\right\rangle \qquad (16)$$

Since $a_k(t)$ is real, from Eqs. (13) and (16) we can get that $\beta_{nk}^A(t)+\widetilde{\omega}_{nk}^A=q^A\pi$; $\beta_{nk}^B(t)+\widetilde{\omega}_{nk}^B=q^B\pi$, and then

$$\beta_{nk}^B(t)=\beta_{nk}^A(t)+q\pi \qquad (17)$$

where q^A, q^B, q are integer, and $\widetilde{\omega}_{nk}^A=\widetilde{\omega}_{nk}^B$ are the phases of $\left\langle E_k^A(t)\,\middle|\,\dot{E}nA(t)\right\rangle$ and $\left\langle E_k^B(t)\,\middle|\,\dot{E}nB(t)\right\rangle$. From Eqs. (12), (14) and (16), we obtain

$$\begin{aligned}\beta_{nk}^B(t) &= -\frac{1}{\hbar}\int_0^t\left(E_n^B-E_k^B\right)dt'\\ &\quad +i\int_0^t\left\{\left\langle E_n^B\,\middle|\,\dot{E}_n^B\right\rangle-\left\langle E_k^B\,\middle|\,\dot{E}_k^B\right\rangle\right\}dt'\\ &= \beta_{nk}^A(t)+\frac{1}{\hbar}\int_0^t\left(E_n^A-E_k^A\right)dt'. \qquad (18)\end{aligned}$$

By Eqs. (17) and (18), we get

$$\frac{1}{\hbar}\int_0^t\left(E_n^A-E_k^A\right)dt'=q\pi. \qquad (19)$$

Eq. (19) is very interesting since it shows the relation between the evolution time and the instantaneous eigenvalues of the Hamiltonian. For any arbitrary system S^A one can always find a corresponding system S^B satisfying Eq. (2), so Eq. (19) is only a result of the Schrödinger equation. If we denote $\overline{\triangle E_{nk}}\equiv\frac{1}{t}\int_0^t\left(E_n^A-E_k^A\right)dt'$ as the average of the $E_n^A-E_k^A$ in the time interval $[0,t]$, Eq. (19) can be expressed as

$$t=\frac{q\pi\hbar}{\overline{\triangle E_{nk}}}. \qquad (20)$$

Eq. (20) means the least evolution time is $\frac{\pi\hbar}{\overline{\triangle E_{nk}}}$(i.e.,$q=1$). Furthermore, if we regard $\overline{\triangle E_{nk}}$ as the energy uncertainty of the system, according to the uncertainty relation $\overline{\triangle E_{nk}}t\sim h$, the time uncertainty is $\frac{h}{\overline{\triangle E_{nk}}}$ which is in the order of the leat evolution time. In fact, if the system undergoes a quantum transition between $|E_n(t)\rangle$ and $|E_k(t)\rangle$ by the evolution according to the Schrödinger equation, the energy of the system has uncertainty of $E_k(t)-E_n(t)$ This can be explained as follows. Suppose the system is in the state $|E_n(t')\rangle$ in the time t', after a evolution from t' to t the system's state becomes $|\psi(t)\rangle$ which is a superposition of the instantaneous eigenstates $|E_n(t)\rangle$ and $|E_k(t)\rangle$(in this case, there is a quantum transition between $|E_n(t)\rangle$ and $|E_k(t)\rangle$). According to quantum mechanics theory, when the system is in the superposition state $|\psi(t)\rangle$ one cannot distinguish whether the system is in the state $|E_n(t)\rangle$ or $|E_k(t)\rangle$. So we can say the system has energy uncertainty $E_k(t)-E_n(t)$. Owing to the uncertainty relation the corresponding time-uncertainty is $\frac{1}{E_k(t)-E_n(t)}$ (We let $h=1$).

How to understand that the least evolution time is the order of time-uncertainty? We can say that any evolution in the time much less than the time-uncertainty $\frac{1}{E_k(t)-E_n(t)}$ will be negligible, namely, the evolution time must not be much less than $\frac{1}{E_k(t)-E_n(t)}$ to produce an effective evolution. Otherwise, we can determinate time parameter with precision more than the time-uncertainty by distinguishing the difference between the states before and after the effective evolution [26], which violates the uncertainty relation. A similar conclusion can also be reached from a different point of view [7]. Let $|\psi(0)\rangle$ and $|\psi(t)\rangle=u(t)|\psi(0)\rangle$ denote the initial state and the state at time t of the system, where $u(t)$ is the evolution operator. The expansion of the $u(t)$ is

$$\begin{aligned} u(t) &= 1-i\int_0^t H(t_1)dt_1 \\ &\quad +\frac{(-i)^2}{2}\int_0^t dt_1\int_0^{t_1} dt_2 H(t_1)H(t_2)+\cdots \end{aligned} \quad (21)$$

Since t is small, we can keep only the first order approximation. let $\overline{H}\equiv\frac{1}{t}\int_0^t H(t_1)dt_1$, then at time t the probability p of finding the system not being in the initial state $|\psi(0)\rangle$ is

$$\begin{aligned} p &= \langle\psi(0)|\,u(t)^+[I-|\psi(0)\rangle\langle\psi(0)|]\,u(t)\,|\psi(0)\rangle \\ &\approx \langle\psi(0)|\,(1+it\overline{H})[I-|\psi(0)\rangle\langle\psi(0)|]\,(1-it\overline{H})\,|\psi(0)\rangle \\ &= \langle\psi(0)|\,\overline{H}^2\,|\psi(0)\rangle\,t^2-\langle\psi(0)|\,\overline{H}\,|\psi(0)\rangle^2\,t^2 \\ &\equiv (\triangle\overline{H})^2t^2, \end{aligned} \quad (22)$$

where $\triangle\overline{H}$, the root mean square deviation of the energy, is the average uncertainty of the energy of the system in the time interval $[0,t]$, its inversion $\frac{1}{\triangle\overline{H}}$ is the uncertainty of the time. If evolution time $t\ll\frac{1}{\triangle\overline{H}}$, then $p\ll 1$. Namely, if the evolution time is much less than the time-uncertainty, the system will stay in the initial state.

From the discussion above, we can conclude that any system has the least effective evolution time (LEET) which is the order of time-uncertainty. $E_k(t)-E_n(t)$ can be regarded as the energy-uncertainty when the system undergoes a transition between the two states $|E_n(t)\rangle$ and $|E_k(t)\rangle$. So the time $\frac{1}{E_k(t)-E_n(t)}$ can be regarded roughly as the least effective evolution time which we denote as T_{LEET}. With those in mind, we can discuss the physical pictures of conditions (1) and (9) easily.

By the basic meaning of the inner product of two vectors in a Hilbert space, we know that $\left\langle E_n(t)\,\middle|\,\dot{E}_m(t)\right\rangle$ is proportional to the amplitude of the probability of the transition from $|E_m(t)\rangle$ to $|E_n(t)\rangle$ in an unit time interval. By equation (8) we know $\int_0^T Re\Big(a_n(t)\,a_m^*(t)\left\langle E_n(t)\,\middle|\,\dot{E}_m(t)\right\rangle\Big)\,dt$ is proportional to the probability of the transition from $|E_n(t)\rangle$ to $|E_m(t)\rangle$) in the time interval $[0,T]$. And then $2T\max\left\{\left|\left\langle E_m(t)\,\middle|\,\dot{E}_n(t)\right\rangle\right|\right\}$ is the maximal probability of the transition from $|E_n(t)\rangle$ to $|E_m(t)\rangle$ in the time interval $[0,T]$. Condition (9) means just that the transition between $|E_n(t)\rangle$ and $|E_m(t)\rangle$ is very small and can be neglected in the whole time interval $[0,T]$. So it is sufficient to assure adiabatic process.

In condition (1), $\frac{\langle E_n(t)|\dot{E}_m(t)\rangle}{E_m(t)-E_n(t)}$ is nothing else but the amplitude of the average probability of the transition between $|E_n(t)\rangle$ and $|E_m(t)\rangle$ in one LEET. The condition $\frac{\langle E_n(t)|\dot{E}_m(t)\rangle}{E_m(t)-E_n(t)}<<1$ for each LEET in the whole time interval $[0,T]$ is necessary for adiabatic process, otherwise, it is possible for the system has an obvious transition between $|E_n(t)\rangle$ and $|E_m(t)\rangle$ in a LEET.

To make the pictures of the necessary condition (1) and the sufficient condition (9) more clear we discuss when the necessary condition becomes sufficient, we investigate the effect of the phases of $a_n(t)$ and $\chi_{nm}(t)$. Let

$$a_n(t)=|a_n(t)|\,e^{-i\int_0^t E_n(t')dt'}; \quad (23)$$

$$\chi_{nm}(t)=|\chi_{nm}(t)|\,e^{i\omega(t)dt}, \quad (24)$$

from Eq. (8), the probability of the transition from the $|E_n(t)\rangle$ to $|E_m(t)\rangle$ is proportional to ϵ_{nm}.

$$\begin{aligned} \epsilon_{nm} &\equiv \int_0^T Re(a_n(t)\,a_m^*(t)\,\chi_{nm})\,dt \\ &= \int_0^T Re\Big(|a_n(t)|\,|a_m^*(t)|\,e^{-i\omega_{nm}(t)t}\,|\chi_{nm}|\,e^{i\omega(t)t}\Big)\,dt \\ &= \int_0^T |a_n(t)|\,|a_m^*(t)|\,|\chi_{nm}|\cos((\omega(t)-\omega_{nm}(t))t)dt \end{aligned} \quad (25)$$

where $\omega_{nm}(t) \equiv \frac{1}{t}\int_0^t E_n - E_m(t')\,dt'$. As shown in [11] in the presence of resonant oscillation, i.e., $\omega(t) = \omega_{nm}(t)$,

$$\begin{aligned}\epsilon_{nm} &= \int_0^T |a_n(t)|\,|a_m^*(t)|\,|\chi_{nm}|\,dt \\ &\le T\max_{t\in[0,T]}|\chi_{nm}|\,.\end{aligned} \tag{26}$$

Suppose that T includes M LEET, i.e., $M \approx \frac{T}{T_{LEET}}$, then

$$\begin{aligned}\epsilon_{nm} &\le T\max_{t\in[0,T]}|\chi_{nm}| = \sum_{i=1}^{M}\max|\chi_{nm}|\,T^i_{LEET} \\ &= \sum_{i=1}^{M}\max\frac{|\chi_{nm}|^i}{E_m(t)^i - E_n(t)^i},\end{aligned} \tag{27}$$

where $T^i_{LEET} = \frac{1}{E_m(t)^i - E_n(t)^i}$ is the i_th LEET. The conditions (1), which means $\max\frac{|\chi_{nm}|^i}{E_m(t)^i - E_n(t)^i} \ll 1$ for each LEET, cannot assure the error of the whole process is small since M may increase as the time T does. But the condition (9) means that $\sum_{i=1}^{M}\max|\chi_{nm}|\,T^i_{LEET} \ll 1$, i.e., the error of the whole process is small, so it is sufficient.

In the absence of resonant oscillation, i.e., $\omega(t) - \omega_{nm}(t) \equiv \omega' \neq 0$, $\epsilon_{nm} = \int_0^T |a_n(t)|\,|a_m^*(t)|\,|\chi_{nm}|\cos\omega' t dt$. This means ϵ_{nm} may not increase as T owing to the different sign of $\cos\omega' t$ in the different LEET. In this case, the adiabatic opproximation holds under condition (1).

It should be noted that if the evolution time T is of the order T_{LEET}, the error of the whole process is small and adiabatic approximation is valid in many cases. For example, consider a simple two-state system as used by Amin [11]. The Hamiltonian of the system is

$$H(t) = -\varepsilon\frac{\sigma_z}{2} - V\sin(\omega_0 t)\,\sigma_x \tag{28}$$

and V is a small positive number. The system's exact instantaneous eigenvalues and eigenstates are

$$E_{0,1} = \pm\frac{1}{2}\Omega; \tag{29}$$

$$|E_{0,1}\rangle = \begin{pmatrix}\alpha^{\pm}\\ \pm\alpha^{\mp}\end{pmatrix} \tag{30}$$

where $\Omega = \sqrt{\varepsilon^2 + 4V^2\sin^2(\omega_0 t)}, \alpha^{\pm} = \sqrt{(\Omega \pm \varepsilon)/2\Omega}$. If $\varepsilon \approx \omega_0$, and the system starts at its ground state, then at time T, the probability of the system ends at the ground state is

$$P_0(t) = |\langle E_0(t)\mid\psi(t)\rangle|^2 \approx \frac{(\cos Vt + 1)}{2}. \tag{31}$$

$E_0 - E_1 = \Omega \approx \varepsilon \approx \omega_0$, so the $T_{LEET} \approx \frac{1}{\omega_0}$. If the evolution time T is of order $\frac{1}{\omega_0}$, then $VT \ll 1$ and $P_0(t) \approx \frac{(\cos Vt+1)}{2} \approx 1$. That means adiabatic approximatoin is valid even in the presence of fast driven oscillations.

In conclusion, we have shown that the evolution time must not be much less than a lower bound which is in the order of the time uncertainty of the system to get an obvious change of the state of the system. The quantitative condition has a clear physical picture: the amplitude of the probability of transition between two levels in each of the least evolution time is small. We also present a new sufficient condition with clear physical meaning. Our results are helpful to clarify the physical images of the some existing conditions for adiabatic approximation and remove the previous doubts on the quantitative condition. A possible interesting topic in the further is: what is the role of the uncertainty relation in the evolution of a quantum system.

We thank Prof. Chengzu Li for helpful discussions. P.-X Chen is very grateful for friendly help of Prof. Ian Walmsley, Dr. Lijian Zhang and the other members in the Walmsley's group when he visited in physics department of Oxford university. This work was supported by NSFC (no:10774192) and FANEDD in China (no 200524).

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